

Endothal
145-73-3 | DTXSID7024081

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 4.10e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.85e-01

Confidence level: 6.84e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Endothal</div> <div>Measured: 5.37e-01</div> <div>Predicted: 4.10e-01</div>	<div>Image not found</div> <div>Butanoic acid, 3-amino-2-hydroxy-</div> <div>Measured: 4.43e-01</div> <div>Predicted: 3.55e-01</div>
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